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A VARIATIONALLY CONSISTENT APPROACH FOR NON-ASSOCIATIVE THERMOPLASTICITY AT FINITE STRAIN

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Abstract. The present paper deals with nonisothermal plasticity at finite strain. Both isotropic and kinematic hardening are included through a non-associative model of Armstrong-Frederick-type. The model proposed in the present contribution is based on the recent works [1, 2]. Within the papers [1, 2], a variationally consistent update was proposed. This update allows computing the state of a thermomechanical solid by minimizing a certain energy potential. The non-trivial extension of [1, 2] to non-associative evolution equations was realized through the introduction of an extended principle of maximum dissipation augmented by a suitable parameterization of evolution equations. The latter formulation was recently presented in [3] within the context of isothermal plasticity. Recently, these authors have extended this approach to non-isothermal plasticity [4]. The predictive capabilities of this model are critically analyzed and demonstrated in the present contribution.

1 INTRODUCTION

Thermomechanically coupled problems were traditionally solved by decoupling the total problem into two sequential steps – the mechanical step in which the temperature is held fixed and the thermal step in which the configuration is fixed. The cornerstone of the aforementioned isothermal step was the radial return method. For capturing the heat dissipation due to plastic deformation, the most common model is the empirical rule of Taylor and Quinney. Unfortunately, this approach can violate the second law of thermodynamics, particularly if cyclic plasticity is considered. A further shortcoming of this approach is that the resulting thermomechanically coupled problem does not show a variational structure, cf. [1]. A variationally consistent reformulation of the thermomechanically coupled problem was recently given in [1]. In the present paper, the formulation presented in [1] is extended to non-associative evolution equations. This extension is based on a modified principle of maximum

dissipation. Concerning isothermal plasticity, such a principle was advocated in [3].

2 A NOVEL VARIATIONALLY CONSISTENT FORMULATION FOR THERMOMECHANICALLY COUPLED PROBLEMS

Without going too much into detail, the variational principle governing the thermomechanically coupled problem as originally proposed in [1] and further elaborated in [4] is defined by the incremental potential

$$I_{inc} = \int_{B_0} \left[E_{n+1} - E_n - \Theta_{n+1}\left(N_{n+1} - N_n\right) + \left[\int_{t_n}^{t_{n+1}} D dt \right] \right] dV \tag{1}$$

$$- \int_{B_0} \Delta t \chi_{n+1} dV - \Delta t P_{\mathbf{F},n+1} + \Delta t P_{\Theta,n+1} \,.$$

Here, E is the internal energy, D is the dissipation, N is the entropy, Θ is the so-called external temperature, χ is a Fourier-type dissipation potential, $P_{\mathbf{F}}$ is a potential defining the mechanical power associated with external forces, P_{Θ} is the counterpart potential for temperature effects, t denotes the time and B_0 is the domain of the considered body. As shown in [1], the state of a deforming body can be described by the stationary conditions of functional (1) for standard dissipative solids (solids fulfilling the normality rule).

For a family of constitutive models showing non-associative evolution equations, the framework proposed in [1] was extended in [4]. This extension is also the focus of the present paper. Conceptually and in line with [3], the idea is an extended principle of maximum dissipation. More precisely, the dissipation functional D, the flow rule and the evolution equations are chosen independently. For enforcing evolution equations different than those implied by the unconstrained principle of maximum dissipation, the concept of pseudo stresses is employed here. Such stresses are denoted as $\tilde{\boldsymbol{\Sigma}}$ in what follows. These stresses are inserted into the desired flow rule. By doing so, all constraints such as plastic incompressibility are automatically fulfilled, cf. [3].

Using the aforementioned parameterization, the unknown deformation φ and the unknown temperature Θ at time t_{n+1} can be computed from the saddle point problem

$$\left(\varphi_{n+1}, \Theta_{n+1}\right) = \arg \inf_{\varphi_{n+1}} \sup_{\Theta_{n+1}} \left\{ \inf_{\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}} I_{inc} \right\}. \tag{2}$$

Here, $\Delta\lambda$ is the integrated plastic multiplier. Problem (2) can be conveniently solved in a staggered fashion. For that purpose, a minimization with respect to the fully locally defined variables is performed first. This gives rise to the local constitutive update

$$\left(\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}\right) = \arg \inf_{\Delta\lambda, \tilde{\boldsymbol{\Sigma}}_{n+1}, N_{n+1}} I_{inc}\big|_{\varphi_{n+1}=const.,\Theta_{n+1}=const.} \,. \tag{3}$$

It can be conveniently solved by applying Newton-type procedures. Subsequently, the stresses follow from the relaxed energy as partial derivatives with respect to the conjugate strain variable.

3 EVOLUTION LAWS AND YIELD FUNCTION

When minimization problem (3) is to be solved, the evolution equations and the stresses have to be specified.

For defining the stresses, the Helmholtz energy is introduced via the classical Legrende-Fenchel transformation

$$\Psi\left(\mathbf{F},\Theta,\boldsymbol{\alpha}\right)=\inf_{N}\left[E\left(\mathbf{F},N,\boldsymbol{\alpha}\right)-N\Theta\right], \tag{4}$$

where $\boldsymbol{\alpha}$ is a set of strain-like internal variables describing plastic deformation. If the set of internal variables is specified as $\boldsymbol{\alpha}=\left\{\mathbf{F}^{p},\boldsymbol{\alpha}_{k},\alpha_{i}\right\}$, the Helmholtz energy reads $\Psi=\left\{\mathbf{F}^{e},\Theta,\boldsymbol{\alpha}_{k},\alpha_{i}\right\}$, where $\mathbf{F}^{e},\mathbf{F}^{p}$ are the elastic and the plastic part of the deformation gradient. Based on Ψ, the stresses are introduced in standard manner, i.e., as derivatives of Ψ with respect to the deformation gradient.

Having defined the stresses, the internal dissipation inequality can be written as (see [4])

$$D_{\text{int}}=\boldsymbol{\Sigma}:\mathbf{L}^{p}+\mathbf{Q}_{k}:\dot{\boldsymbol{\alpha}}_{k}+Q_{i}\dot{\alpha}_{i}\geq 0, \tag{5}$$

where $\mathbf{L}^{p}$ is plastic velocity gradient, $\boldsymbol{\Sigma}$ is the Mandel stress tensor and $\mathbf{Q}_{k},Q_{i}$ are stress-like internal variables conjugate to the strain-like kinematic hardening variable $\boldsymbol{\alpha}_{k}$ and the strain-like isotropic hardening variable α_{i}, respectively.

With (5) the temperature evolution can be defined from the balance of energy. After a straightforward computation it is given by

$$c\dot{\Theta}=\rho_{0}Q_{\Theta}-\text{DIV}\mathbf{H}+D_{\text{int}}+\Theta\partial^{2}_{\Theta\mathbf{F}^{e}}\Psi:\dot{\mathbf{F}}^{e}, \tag{6}$$

where c is the heat capacity at constant strain, $\mathbf{H}$ is the outward heat flux vector and Q_{Θ} is heat source per unit mass. The last term governs thermoelastic heating and it is frequently neglected.

According to (5), the internal dissipation depends crucially on the considered state. For distinguishing between plastic and elastic deformation, the by now classical a yield function is considered. In the present paper, this yield function is assumed to be of the type

$$\phi\left(\boldsymbol{\Sigma},\mathbf{Q}_{k},Q_{i},\Theta\right)=\boldsymbol{\Sigma}^{eq}\left(\boldsymbol{\Sigma}-\mathbf{Q}_{k}\left(\boldsymbol{\alpha}_{k}\right)\right)-Q_{i}\left(\alpha_{i}\right)-Q_{0}^{eq}\left(\Theta\right)\leq 0. \tag{7}$$

Here, the initial yield stress $Q_{0}^{eq}\left(\Theta\right)$ is chosen as temperature dependent. The function $\boldsymbol{\Sigma}^{eq}$ defining the shape of the yield function is assumed to be convex and positively homogenous function of degree one, i.e.,

$$\boldsymbol{\Sigma}^{eq}\left(c\left(\boldsymbol{\Sigma}-\mathbf{Q}_{k}\right)\right)=c\boldsymbol{\Sigma}^{eq}\left(\boldsymbol{\Sigma}-\mathbf{Q}_{k}\right). \tag{8}$$

Finally, the evolution equations are defined. For that purpose and in line with the framework of generalized standard solids, a plastic potential is introduced. In the present paper, this potential is of the type

$$g\left(\boldsymbol{\Sigma},\mathbf{Q}_{k},Q_{i},\Theta\right)=\phi\left(\boldsymbol{\Sigma},\mathbf{Q}_{k},Q_{i},\Theta\right)+\overline{\phi}\left(\mathbf{Q}_{k}\right). \tag{9}$$

The evolution equations are gradients of g. More precisely,

$$\mathbf{L}_{\boldsymbol{\alpha}}^{p} = \lambda \partial_{\boldsymbol{\Sigma}} \bar{\phi}, \quad \dot{\mathbf{Q}}_k = -\dot{\boldsymbol{\alpha}}^{p} + \lambda \partial_{\mathbf{Q}_k} \bar{\phi}, \quad \dot{\alpha}_i = -\lambda \,. \tag{10}$$

(10) is supplemented by the standard Karush-Kuhn-Tucker conditions.

In the case of a von Mises yield function and applying the concept of pseudo stresses $\tilde{\boldsymbol{\Sigma}}$, (10) can be re-written as

$$\mathbf{L}_{\boldsymbol{\alpha}}^{p} = \lambda \frac{\mathrm{Dev}\tilde{\boldsymbol{\Sigma}}}{\left\| \mathrm{Dev}\tilde{\boldsymbol{\Sigma}} \right\|}, \quad \dot{\mathbf{Q}}_k = -\lambda \frac{\mathrm{Dev}\tilde{\boldsymbol{\Sigma}}}{\left\| \mathrm{Dev}\tilde{\boldsymbol{\Sigma}} \right\|} + \lambda \partial_{\mathbf{Q}_k} \bar{\phi}, \quad \dot{\alpha}_i = -\lambda \,. \tag{11}$$

If the yield function is now combined with the dissipation inequality (5), the internal dissipation takes the form

$$D_{\mathrm{int}} \overset{\phi=0}{=} \lambda Q_0^{eq} + \lambda \mathbf{Q}_k : \frac{\partial \bar{\phi}}{\partial \mathbf{Q}_k} \geq 0 \,. \tag{15}$$

Accordingly, the second law of thermodynamics is automatically fulfilled, if the plastic potential (9) is convex. That can be guaranteed by using a convex yield function (which is the case for the von Mises model) and a convex function $\bar{\phi}$.

4 EXAMPLE AND CONCLUSIONS

For demonstrating the efficiency of the discussed framework, the cyclic tension test is numerically analyzed, cf. [3, 5]. In line with [1, 2] adiabatic conditions are considered. The material response is defined by a Helmholtz energy of the type

$$\Psi = W\left(\bar{\mathbf{C}}^{e}\right) + U(J) + T(\Theta) + M(J,\Theta) + \Psi^{p}\left(\boldsymbol{\alpha}_k\right), \tag{16}$$

where the potential $W\left(\bar{\mathbf{C}}^{e}\right)$ defining the elastic deviatoric response as a function of the deviatoric elastic right Cauchy-Green tensor $\bar{\mathbf{C}}^{e}$, the potential $U(J)$ depending on the Jacobian determinant of the deformation gradient characterizing the elastic volumetric response, the part $T(\Theta)$ associated with thermal effects, the part $M(J,\Theta)$ related to thermoelastic effects and the potential $\Psi^{p}\left(\boldsymbol{\alpha}_k\right)$ corresponding to kinematic hardening are chosen as

$$W\left(\bar{\mathbf{C}}^{e}\right) = \frac{1}{2}\mu\left[\mathrm{tr}\left(\bar{\mathbf{C}}^{e}\right) - 3\right], \; U(J) = \frac{1}{2}\kappa\left[\frac{1}{2}\left(J^2 - 1\right) - \ln J\right], \tag{17}$$

$$T(\theta) = c_0\left[\left(\Theta - \Theta_0\right) - \Theta \ln\frac{\Theta}{\Theta_0}\right], \; M(J,\Theta) = \left(\Theta - \Theta_0\right)\left[-3\alpha U'(J)\right], \; \Psi^{p} = \frac{1}{2}c\boldsymbol{\alpha}_k : \boldsymbol{\alpha}_k \,.$$

Thermal softening is accounted for by a temperature-dependent initial yield stress of type

$$Q_0^{eq}(\theta) = y_0(\theta_0)\left[1 - \omega_0\left(\theta - \theta_0\right)\right]. \tag{18}$$

The plastic response is completed by a von Mises yield function

$$\phi\left(\boldsymbol{\Sigma},\mathbf{Q}_k,\Theta\right)=\left\|\mathrm{Dev}\boldsymbol{\Sigma}-\mathbf{Q}_k\right\|-Q_0^{eq} \tag{19}$$

including kinematic hardening and the evolution equations and the flow rules are defined by the gradients of the convex plastic potential

$$g\left(\boldsymbol{\Sigma},\mathbf{Q}_k,\Theta\right)=\phi\left(\boldsymbol{\Sigma},\mathbf{Q}_k,\Theta\right)+\bar{\phi}\left(\mathbf{Q}_k\right);\quad \bar{\phi}\left(\mathbf{Q}_k\right)=\frac{1}{2}\frac{b}{c}\left\|\mathbf{Q}_k\right\|^2 \tag{20}$$

with respect to their dual variables. Finally, the thermal problem is governed by the Fourier dissipation potential

$$\chi=\frac{1}{2}k\mathrm{GRAD}\,\Theta\cdot\mathrm{GRAD}\,\Theta\,. \tag{21}$$

The material parameters used in the numerical simulations are summarized in Tab. 1.

Table 1: Material parameters

μ, GPa	κ, GPa	α, GPa	b
80	173.333	$1.15\cdot10^{-5}$	8.5
c, GPa	y_0, MPa	c_0, N/mm^{2}K	ω_0, K^{-1}
1.9	244.95	3.7518	0.002

Within the variational framework, the part of the mechanical dissipation which is transferred to heat is consistently governed by the first law of thermodynamics. However, by assuming the classical Taylor-Quinney coupling, a Taylor-Quinney factor can be computed as a post-processing step, cf. [1]. The respective results for the first loading stage are shown in Fig. 1. Accordingly and as already mentioned in [1], the assumption of a constant factor is not in line with the first law of thermodynamics. More precisely, the evolution of this factor is highly non-linear. That confirms that the classical Taylor-Quinney assumption is not valid in general and can usually only be justified by a mean value of the more complex and physically more sound evolution shown in Fig. 1. Such problems can be conveniently and naturally solved by using the advocated variationally consistent thermomechanically coupled model.

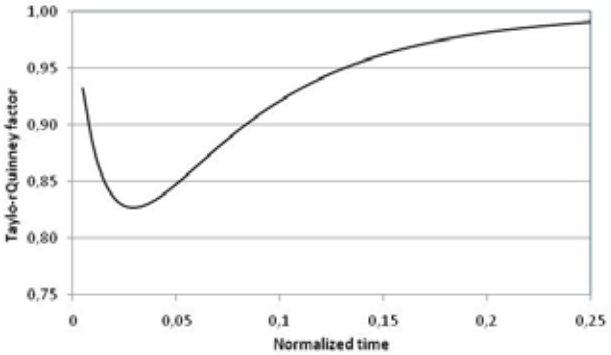

Figure 1: Evolution of the Taylor-Quinney factor as predicted by the variationally consistent model

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